### Analysis of Packing Function Solutions for Monomeric **Proteins**

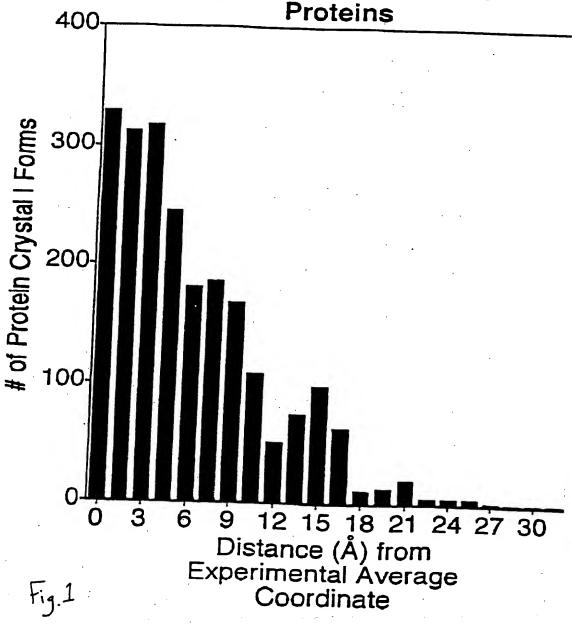
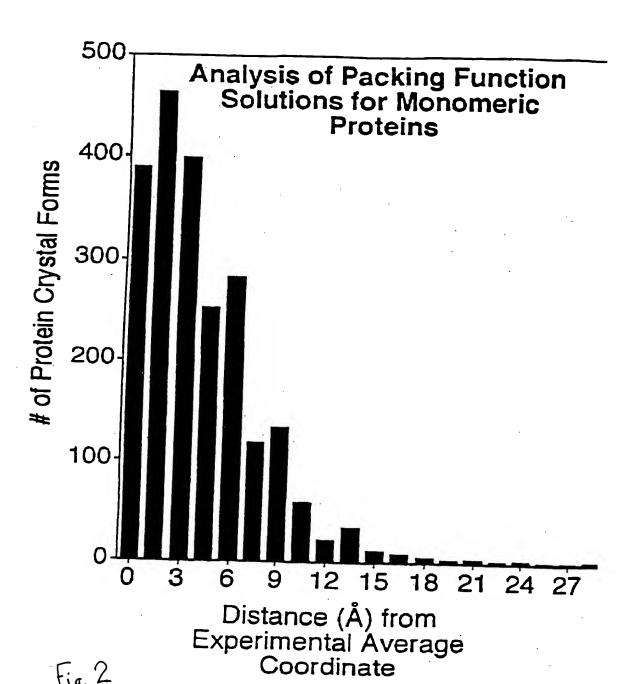


Fig. 2



START: For Use with a Radial Correction or Modes 1& 2 (cont'd) with Modes 5 thru 7: Cycle Set Up F r Each Choice (mstop) of Gct Parallelization Stopping Value for the SHSB Fractionalization m index Matrix Initialize Update Correlation Partition the List Constants and Exponentiation of Fourier Indices Sine/Cosine Tables Factor Between Processor(s) If there is a Prior Model Input 1 & Convert Each Fourier Initialize the List of (On cycles after the 1st cycle i Index (hkl) to Polar of the 1st run of the program): Fourier Indices (hkl) Coordinates & Get On Cycles After the Its Bessel Argument 1st value of mstop Get Biggest Sphere Update the File # for Get the FT of a Without Overlap the Calculated FT Crystalline Unit Cell of Symmetry Mates Filled with Symmetry For Each input SHSB Model Related Spheres Convert the File # Calculate a Radial Input 2 & the Model # Correction Factor to a File Name for Each "n" Index Read Input Confirm FT & SHSB coefs Calculation Mode Calculation Mode-Specific Routines: of the Prior Model If there is No Prior Model: Modes 1 & 2 Initialize (Unphased Diffraction Amplitudes to Tables of Spherical Model the Crystal as Phased FT of SHSB-modeled Unit Cell) Bessel Functions and a Crystalline Unit Cell Bessel Function 0's Filled with Symmetry Related Spheres Mode-Specific Determine Limits -----Input Gct a Starting Value on 1 & m indices and (msus) for the SHSB on n indices at each l m Index for the Next Get Input File # for Packet of m Values For modes 5 thru 7: Calculated FT, if Rend expected SHSB Update the Model here is a Prior Model coefficient & by Adjusting the deviation values Contributions of Initialize Correlation each SHSB function Exponentiation for each lmn index in Factor the m-packet from 'insus' to 'mstop'

Flow Chart for the Main Driver Program for "faizer": Options to compute a the PI of a SHSB Model of Crystal

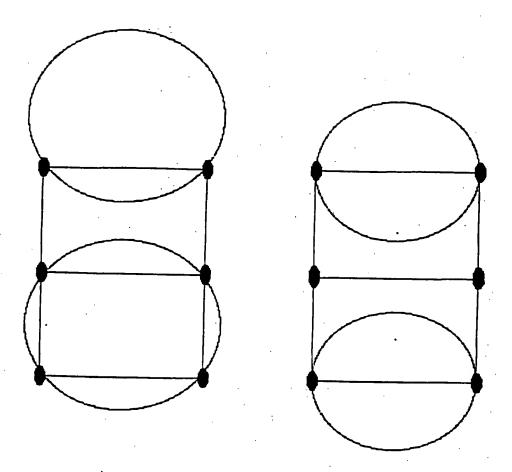


Figure A schematic example: Two choices for filling the same portion of a crystal unit cell from an orthorhombic Spacegroup. Although the spheres on the right are smaller than those on the left, for some crystals, the local maximum in the packing on the right wold be the packing of maximal consistency with the crystallographic data.

Figure 4.

Initialize Fractionalization Matrix

Initialize the Equal Partitioning of the Fourier (hkl) Index between Processors

On 1st Cycle of 1st Run:

Prescale Observed
Diffraction to that
of a Unit Cell of
Spheres

Define the First SHSB Index Triplet (Imn) for which to Consider Model |F|'s

Initialize for Indexby-Index Update of Origin-Centered SHSB Basis Function

Modes 4 & 5 only: Initialize Buffers for Cumulative Update of Fourier Representation

Initialize Pointers to Stored Fourier Representations of Model and of Basis

Mode 3 only: Get File Name from File # & Open It to Let SHSB Coefs, be Read For each "m" Index (0 to maximum "m")

For Each hkl in this Partition:

Update "m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

For each "!" Index (present "m" to maximum "!")

For Each hkl in this Partition:

Update "I,m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

For each "n" Index (1 to maximum "n" for each "!")

> For Each hkl in this Partition:

Update "n" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

Depending on Mode: Choose the # of Passes and # of Presumed Phase Angles Needed for the SHSB coef, with this SHSB index (Imn)

Set the Presumed Amplitude of the Origin-Centered SHSB Basis Function

### **FIRST PASS:**

Initialize Registers: Overall Comparison of Correlation Coef. & Other Statistics

Renitialize Pointers to Storage Sites for Fourier Representations of the Full-Unit-Cell SHSB Basis

Parallel Processor Version:

Set # of calculations to: (# of presumed values of SHSB coef. 's phase)

(# of stored accumulated SHSB models for trial combination with this new SHSB component)

Given: # of processors # of hkl partitions # of calculations Get: # of required rounds of trial combinations

For each round of trial combination on this processor

Single Processor Version:
(Outer Loop)

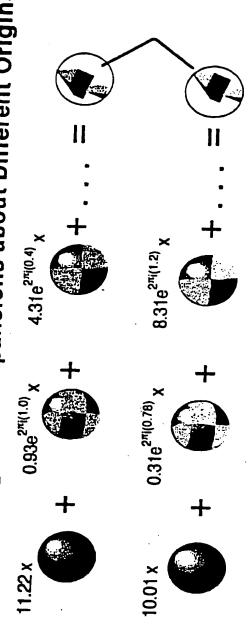
For each presumed value of the SHSB coef.'s phase

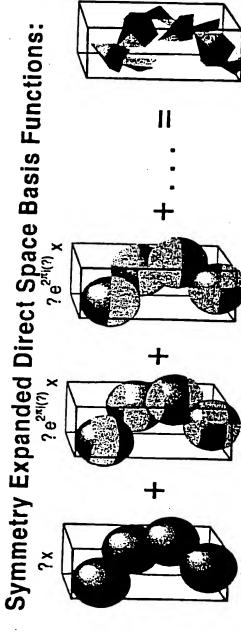
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Initialize Registers: Angular Comparison of Correlation Coef. & Other Statistics

Fig. 5

# Identical Image from Expansions about Different Origins:

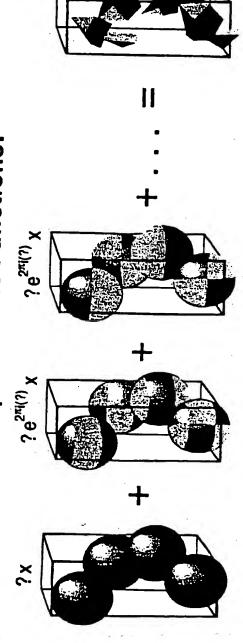




With a properly chosen origin, 45-55% of the unit cell can be expanded. (Most protein crystals are > 45% solvent.)

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## Component Direct Space Basis Functions:



## Component Fourier Transforms:

$$a_{001}F_{solo}^{001}(hkl) + a_{211}F_{solo}^{211}(hkl) + a_{111}F_{solo}^{111}(hkl) + \dots = F_{obs}(hkl)$$

 $a_{001} = \sum_{hkl} F^*_{solo}$  (hkl)  $F_{obs}$ (hkl) [presume  $\phi = 0.00$  to start]

$$F_{\text{accum}}(\text{hkl}) = a_{001} F_{\text{solo}}^{001}(\text{hkl})$$

 $a_{211} = \sum_{hkl} F^*_{solo}(hkl) (|F_{obs}(hkl)| - |F_{accum}(hkl)|) e^{2m \phi''(hkl)}$ 

$$F_{\text{accum}}(hkl) = F_{\text{accum}}(hkl) + a_{211}F_{\text{solo}}^{211}(hkl)$$



